

Self-Adjoint Extensions of the Pauli Equation in the Presence of a Magnetic Monopole

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Abstract

We discuss the Hamiltonian for a nonrelativistic electron with spin in the presence of an abelian magnetic monopole and note that it is not self-adjoint in the lowest two angular momentum modes. We then use von Neumann's theory of self-adjoint extensions to construct a self-adjoint operator with the same functional form. In general, this operator will have eigenstates in which the lowest two angular momentum modes mix, thereby removing conservation of angular momentum. However, consistency with the solutions of the Dirac equation limits the possibilities such that conservation of angular momentum is restored. Because the same effect occurs for a spinless particle with a sufficiently attractive inverse square potential, we also study this system. We use this simpler Hamiltonian to compare the eigenfunctions corresponding to a particular self-adjoint extension with the eigenfunctions satisfying a boundary condition consistent with probability conservation.

I. INTRODUCTION

In this article, we first examine the Pauli Equation for an electron in the field of a magnetic monopole. This equation has appeared in the literature before, and it is well known

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that an extension is needed to make the Hamiltonian self-adjoint in the $j = 0$ sector [1]. What seems to have gone unnoticed is that, for $eg = \frac{1}{2}$, the domain to be extended includes the $j = 1$ sector as well. With the inclusion of this sector, the structure of the extensions becomes richer, and the number of parameters required to describe them jumps from 1 to 16. While the parameters may be chosen to be consistent with angular momentum conservation, this is not required: a pure incoming s-wave can come out with a p-wave component, even though the functional form of the Hamiltonian is spherically symmetric. However, if we require our states to match the states of the Dirac equation in the nonrelativistic limit, we will only have 1 free parameter, and angular momentum will be conserved. To better understand the effect of the extension parameters and their relation to angular momentum conservation, we also consider a simpler Hamiltonian of the form

$$H = -\frac{1}{2\mu}\nabla^2 - \frac{c}{2\mu r^2}, \quad (1)$$

where c is an arbitrary constant. (Spin is not essential to this discussion and is omitted.) This Hamiltonian has all the essential features of the monopole Hamiltonian, so we can use it to investigate how the extension parameters arise. To accomplish this, we look at this Hamiltonian in 3-space minus a sphere of radius r_0 around the origin. We compare the results of imposing a boundary condition consistent with probability conservation with the results of creating a self-adjoint extension. Finally, we compare the case of a nonzero radius r_0 with that of a zero radius r_0 .

II. PAULI EQUATION

Working in units where the speed of light and Planck's constant are both equal to one, the Hamiltonian for an electron (with spin) in an electromagnetic field is

$$H = \frac{\vec{\pi}^2}{2\mu} - \frac{e}{2\mu}\vec{\sigma} \cdot \vec{B}, \quad (2)$$

where $\vec{\pi}$ is the kinematic momentum $\vec{p} - e\vec{A}$, \vec{A} is the vector potential, and \vec{B} is the magnetic field. For a point magnetic monopole of strength g sitting at the origin [2], we have

$$\vec{A} = \frac{g(1 - \cos \theta)}{r \sin \theta} \hat{\phi} \quad (3)$$

$$\vec{B} = \frac{g\hat{r}}{r^2} \quad (4)$$

$$H = \frac{\vec{\pi}^2}{2\mu} - \frac{eg\vec{\sigma} \cdot \hat{r}}{2\mu r^2}, \quad (5)$$

where we have chosen a particular gauge to determine \vec{A} . Using $\vec{L} = \vec{r} \times \vec{\pi} - eg\hat{r}$, the Hamiltonian can be rewritten as

$$H = \vec{\pi} \cdot \vec{r} \frac{1}{2\mu r^2} \vec{r} \cdot \vec{\pi} + \frac{\vec{L}^2 - e^2 g^2 - eg\vec{\sigma} \cdot \hat{r}}{2\mu r^2}. \quad (6)$$

Here \vec{L} is the orbital angular momentum satisfying $[L^i, V^j] = i\epsilon^{ijk}V^k$ for any spin-independent vector operator. Note that $[L^i, H] \neq 0$. The angular momentum operator that commutes with H is the total angular momentum $\vec{J} = \vec{L} + \frac{1}{2}\vec{\sigma}$. In appendix I, (6) is shown to simplify to

$$H = -\frac{1}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r + \frac{K(K+1)}{2\mu r^2} \quad (7)$$

with the further definition

$$K = -1 - \vec{r} \times \vec{\pi} \cdot \vec{\sigma} \quad (8)$$

[3]. We can find simultaneous eigenstates of K , J^2 , and J_z involving only angular variables. Such “monopole harmonics” will be denoted by $\Omega_{\kappa m}(\theta, \phi)$ and satisfy

$$K\Omega_{\kappa m} = \kappa\Omega_{\kappa m} \quad (9)$$

$$J^2\Omega_{\kappa m} = j(j+1)\Omega_{\kappa m} \quad (10)$$

$$J_z\Omega_{\kappa m} = m\Omega_{\kappa m} \quad (11)$$

$$\int d\Omega |\Omega_{\kappa m}(\theta, \phi)|^2 = 1 \quad (12)$$

where j takes on the values $0, 1, 2, \dots$ and κ is related to j by

$$\kappa = \pm\sqrt{j(j+1)} \quad (13)$$

for $eg = \frac{1}{2}$. (More generally, $\kappa = \pm\sqrt{(j + \frac{1}{2})^2 - e^2g^2}$ with $j = eg - \frac{1}{2}, eg + \frac{1}{2}, \dots$. See appendix I.) Note that for $j > 0$ (or $j > eg - \frac{1}{2}$ in the general case), there are two sets of m -multiplets for each value of j , one corresponding to $\kappa > 0$, and one corresponding to $\kappa < 0$. In terms of Bessel functions and the monopole harmonics, the $E > 0$ solutions to the eigenvalue equation $H\psi = E\psi$, are

$$\Psi_N^{\kappa m E} = r^{-\frac{1}{2}} J_{\nu_\kappa}(\lambda r) \Omega_{\kappa m}(\theta, \phi) \quad (14)$$

$$\Psi_S^{\kappa m E} = r^{-\frac{1}{2}} Y_{\nu_\kappa}(\lambda r) \Omega_{\kappa m}(\theta, \phi) \quad (15)$$

$$\lambda = \sqrt{2\mu E}, \quad \nu_\kappa = \left| \kappa + \frac{1}{2} \right|$$

and the $E < 0$ solutions are

$$\Psi_B^{\kappa m E} = r^{-\frac{1}{2}} K_{\nu_\kappa}(\lambda r) \Omega_{\kappa m}(\theta, \phi) \quad (16)$$

$$\lambda = \sqrt{-2\mu E}, \quad \nu_\kappa = \left| \kappa + \frac{1}{2} \right|.$$

(There is another set of $E < 0$ solutions which has I_{ν_κ} instead of K_{ν_κ} , but they grow exponentially at large distances and need not be considered.) At this point we mention that any dependence on the gauge is contained entirely in the form of the $\Omega_{\kappa m}$. The radial part of these solutions and the eigenvalues of the operators are left invariant under a gauge transformation. The set (14) (N for Nonsingular) of solutions vanishes at the origin, while the sets (15) (S for Singular) and (16) (B for bound) are singular at the origin. Although the Ψ_N are not square integrable over all space, they can be δ -function normalized and are square integrable over any finite region. However, the Ψ_S and Ψ_B are only normalizable (δ -function normalizable in the case of the Ψ_S) when $\nu_\kappa < 1 \Leftrightarrow \kappa = 0, -\sqrt{2}$ (i.e. for the $j = 0$ singlet and one $j = 1$ triplet). If $\nu_\kappa \geq 1$, the Ψ_S and Ψ_B are not square integrable over any region containing the origin. (The cutoff $\nu_\kappa = 1$ is equivalent to a coefficient of $\kappa(\kappa + 1) = \frac{3}{4}$ for the $\frac{1}{r^2}$ term in (7). This coefficient is a general cutoff for a $\frac{1}{r^2}$ potential [6] [7] [8].) It is tempting to let the Hamiltonian operator (7) act on all linear combinations of the normalizable (including δ -function normalizable) solutions. However, this is incompatible with the Hermiticity condition $(H\phi, \psi) = (\phi, H\psi)$ for all ϕ, ψ in the

domain of H . Furthermore, we seek a Hamiltonian which is not only Hermitian, but also self-adjoint, for only then are its eigenfunctions complete. At this point, we need to become more precise in our usage of the term operator, from now on including the domain of an operator as part of the operator's definition. Precise definitions of Hermitian and self-adjoint will be employed, and can be found in appendix II. To start with, let H_1 be the operator given functionally by H in (7), and defined on all functions ψ in the Hilbert space such that $H\psi$ is in the Hilbert space. We expect the Hamiltonian to be Hermitian; however,

$$(H_1\psi, \phi) = (\psi, H_1\phi) + \lim_{r \rightarrow 0} \frac{1}{2\mu} \int r^2 d\Omega \left(\frac{\partial \psi^*}{\partial r} \phi - \psi^* \frac{\partial \phi}{\partial r} \right) \quad (17)$$

from integration by parts, so H_1 is not Hermitian. Next, define H_2 to be the operator identical to H_1 except that the domain is further restricted to

$$\left\{ \phi \in \text{dom}(H_1) \left| \lim_{r \rightarrow 0} \int r^2 d\Omega \left(\frac{\partial \psi^*}{\partial r} \phi - \psi^* \frac{\partial \phi}{\partial r} \right) = 0 \text{ for all } \psi \in \text{dom}(H_1) \right. \right\}. \quad (18)$$

By comparing (17) with (18), H_2 is seen to be Hermitian. In other words, the domain of H_2 is the set of ϕ in the domain of H_1 such that

$$(\psi, H_2\phi) = (H_1\psi, \phi) \quad (19)$$

for all ψ in the domain of H_1 , which means that $H_2^\dagger = H_1$. (H_1 is the adjoint of H_2 .) Since the domain of H_1 is larger than that of H_2 , H_2 is not self-adjoint; however, the domain of H_2 can be extended through a method of von Neumann to create an operator that is self-adjoint. According to the von Neumann theory of self-adjoint extensions, we need to look at the number n_+ of normalizable solutions to the equation $H_1\phi_+ = +i\mu\phi_+$ and the number n_- of normalizable solutions to the equation $H_1\phi_- = -i\mu\phi_-$. (Note that the use of μ is arbitrary and chosen only to provide the correct units. Any positive real constant may be used instead.) We can index these solutions and denote them by ϕ_\pm^i , where i ranges from 1 to n_\pm . If $n_+ = n_- \equiv n$, then H_2 can be made self-adjoint by introducing the n vectors $\phi^i = \phi_+^i + U_j^i \phi_-^j$ into its domain, where U is an arbitrary unitary $n \times n$ matrix (with n^2 real parameters). Thus, a general element of the domain of the extended Hamiltonian, H_U , is of

the form $\sum c_i \phi^i + \tilde{\phi}$, where $\tilde{\phi}$ is in the domain of H_2 . (The reader can check that the extended Hamiltonian satisfies the self adjointness criterion of appendix II.) For the monopole, the domain of H_2 consists of those functions in the domain of H_1 that vanish at the origin at least as fast as $r^{1/2}$. Then, the normalized solutions to $H_1 \phi_{\pm} = \pm i \mu \phi_{\pm}$ are

$$\phi_{\pm}^{jm} = \sqrt{\frac{8\mu^2 \cos(\nu_{\kappa} \pi/2)}{\pi}} r^{-1/2} K_{\nu_{\kappa}}((1 \mp i)\mu r) \Omega_{\kappa m}, \quad (20)$$

$$j = 0, \kappa = 0, m = 0 \text{ or } j = 1, \kappa = -\sqrt{2}, m = 0, \pm 1.$$

There are 4 of each, so von Neumann's Theorem tells us that we need $4^2 = 16$ parameters to describe each extension. Given 16 parameters in the form of a unitary matrix $U_{j'm'}^{jm}$, ($j, j' = 0, 1$; $m = -j, \dots, j$; $m' = -j', \dots, j'$), the Hamiltonian can be made self-adjoint by introducing the 4 vectors

$$\phi^{jm} = \phi_+^{jm} + U_{j'm'}^{jm} \phi_-^{j'm'} \quad (21)$$

into its domain. (On a cautionary note: The superscripts jm on the ϕ^{jm} should be considered merely labels. The states ϕ^{jm} defined above and the Ψ_E^{jm} defined below are not necessarily eigenstates of angular momentum.) The ϕ^{jm} are not energy eigenstates; however, for each ϕ^{jm} and for each positive energy eigenvalue E , there exists one energy eigenstate, Ψ_E^{jm} , that differs from ϕ^{jm} by an element in the domain of H_2 . When $U_{j'm'}^{jm}$ is diagonal, the Ψ_E^{jm} are simultaneous eigenfunctions of J^2 , J_z , and H_U , but in general this is not the case: The Ψ_E^{jm} will be eigenfunctions of H_U only, since the simultaneous eigenstates of H_1 , J^2 , and J_z corresponding to $j = 0, 1$ are not in the domain of H_U . Similarly, not all of the eigenstates of J^2 and J_z will be eigenstates of H_U . In other words, a pure angular momentum eigenstate with $j = 0, 1$ will in time evolve as a superposition of states with mixed angular momenta. Thus, angular momentum is not conserved for general U . Now we can construct the energy eigenstates. Because the Ψ_E^{jm} differ by ϕ^{jm} by an element in the domain of H_2 , which vanishes at the origin at least as fast as $r^{\frac{1}{2}}$, we only need to consider the behavior of the solutions (14), (15), and (16) at the origin. To get a particular energy eigenstate, pick a value of energy E and a particular ϕ^{jm} . Then, look at its behavior and the behavior of the

above solutions for small r . Any linear combination of solutions whose small r behavior matches the small r behavior of the particular ϕ^{jm} (up to a part that vanishes at least as fast as $r^{\frac{1}{2}}$) is an eigenvalue of the self-adjoint operator H_U . For positive values of E , there is precisely one energy eigenstate for each ϕ^{jm} . However, most negative values of E fail to yield an eigenstate. When we try to match the solution to ϕ^{jm} , we derive the following relation between the energy E and the diagonal matrix element U_{jm}^{jm} :

$$E = -\mu \left[\frac{1 + i^{\nu_\kappa} U_{jm}^{jm}}{i^{\nu_\kappa} + U_{jm}^{jm}} \right]^{\frac{1}{\nu_\kappa}}, \quad (22)$$

where, as before, $\nu_\kappa = \left| \kappa + \frac{1}{2} \right|$ and $\kappa = \pm \sqrt{j(j+1)}$. (Specifically, we are only interested in $\kappa = 0$ for $j = 0$ and $\kappa = -\sqrt{2}$ for $j = 1$.) For the bound state to exist, we require that E be real and negative. The reality condition requires $|U_{jm}^{jm}|^2 = 1$. Since U is unitary, this requires the the row and column corresponding to j and m consist entirely of zeros, except for the diagonal element, which must be of the form $e^{i\theta}$, where θ is real. (Note that this also implies that the bound state must be an angular momentum eigenstate.) This allows us to simplify (22) to

$$E = -\mu \left[\frac{\cos(\pi\nu_\kappa/2) + \cos(\theta)}{1 + \cos(\theta - \pi\nu_\kappa/2)} \right]^{\frac{1}{\nu_\kappa}}. \quad (23)$$

So we see that we also have the additional condition on the diagonal element:

$$\cos(\theta) \geq -\cos(\pi\nu_\kappa/2). \quad (24)$$

There exists one bound state for each such row; therefore, there can be anywhere from zero to four bound states, depending on the particular self-adjoint extension chosen. Now we compare our results with a similar treatment for the Dirac equation that has already appeared in the literature [9] [10]. We work with the Dirac Hamiltonian

$$H = \vec{\alpha} \cdot \vec{\pi} + \beta\mu \quad (25)$$

and in a basis where

$$\vec{\alpha} = \begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (26)$$

and $\vec{\sigma}$ are the Pauli matrices. The advantage of this basis is that the Dirac spinor can be separated into upper and lower bispinors, where the lower bispinor is dropped in the nonrelativistic limit. When appropriately separated, the eigenvalue equation $H\psi = E\psi$ becomes

$$\psi = \begin{pmatrix} f^{\kappa m E}(r)\Omega_{\kappa m} \\ g^{\kappa m E}(r)\Omega_{-\kappa m} \end{pmatrix} \quad (27)$$

$$(\mu - E)f^{\kappa m E} - i(\partial_r + \frac{1 - \kappa}{r})g^{\kappa m E} = 0 \quad (28)$$

$$i(\partial_r + \frac{1 + \kappa}{r})f^{\kappa m E} + (\mu + E)g^{\kappa m E} = 0. \quad (29)$$

Solving for $f^{\kappa m E}$, we get the familiar solutions for $E > \mu$

$$f_N^{\kappa m E} = r^{-\frac{1}{2}}J_{\nu_\kappa}(\lambda r) \quad (30)$$

$$f_S^{\kappa m E} = r^{-\frac{1}{2}}Y_{\nu_\kappa}(\lambda r) \quad (31)$$

$$\lambda = \sqrt{E^2 - \mu^2}, \quad \nu_\kappa = \left| \kappa + \frac{1}{2} \right|$$

and for $E < \mu$

$$f_B^{\kappa m E} = r^{-\frac{1}{2}}K_{\nu_\kappa}(\lambda r) \quad (32)$$

$$\lambda = \sqrt{\mu^2 - E^2}, \quad \nu_\kappa = \left| \kappa + \frac{1}{2} \right|.$$

These are the same solutions as for the Pauli equation, except that λ has the different expression above. However, if we let $E = \mu + E'$ and identify E' with the nonrelativistic energy, we get $\lambda = |2\mu E' + E'^2|^{1/2} \longrightarrow |2\mu E'|^{1/2}$ in the nonrelativistic $E' \ll \mu$ limit, and we recover the solutions to the Pauli equation in this limit. One additional difference between the solutions to the Pauli and Dirac equations is that we now have an additional function $g^{\kappa m E} = -i(\partial_r + (1 + \kappa)r^{-1})f^{\kappa m E}/(\mu + E)$, which we require to be square integrable

over a finite region containing the origin. One may easily check for $\kappa = -\sqrt{2}$ that $g_S^{\kappa m E}$ is not square integrable over this region, even though $f_S^{\kappa m E}$ is. Thus, we no longer have the singular solution for $\kappa = -\sqrt{2}$ as we did in the Pauli case above. When we look for self-adjoint extensions, we find that we no longer need an extension for the $j = 1$ sector; only the $j = 0$ sector requires an extension. Thus, angular momentum modes may not mix; furthermore, we only need one parameter to specify the extension. From another point of view, consistency with the nonrelativistic limit of the Dirac equation requires us to fix 15 of the 16 parameters of the Pauli equation.

III. GENERAL $\frac{1}{R^2}$ POTENTIAL

The Pauli equation in the presence of a magnetic monopole is just one example of a Hamiltonian where the choice of a self-adjoint extension can lead to non-conservation of angular momentum. Looking at the form of (7), we can see that the same essential behavior can be obtained from a spinless particle with a sufficiently attractive inverse square potential, as in (1). Analysis of this new Hamiltonian is simple and analagous to the analysis of the magnetic monopole. Similarly, the arguments in this section can be modified to include the monopole Hamiltonian or any similar Hamiltonian that needs an extension. With this simpler Hamiltonian, we can investigate how the extension parameters arise. To do this, consider a space with a sphere of radius r_0 and centered around the origin removed. We impose conservation of probability at the boundary and seek a relation between the extension parameters and the boundary conditions. Now, consider a spinless particle governed by the Hamiltonian (1), whose functional form is given by (using $\vec{L} = -i\vec{r} \times \vec{\nabla}$)

$$H = -\frac{1}{2\mu} \frac{1}{r} \frac{d^2}{dr^2} r + \frac{-c + L^2}{2\mu r^2}, r \geq r_0. \quad (33)$$

This Hamiltonian has appeared in the literature before. [6] The solutions to $H\psi = E\psi$ are

$$\Psi_N^{lmE} = r^{-\frac{1}{2}} J_{\nu_l}(\lambda r) Y^{lm}(\Omega) \quad (34)$$

$$\Psi_S^{lmE} = r^{-\frac{1}{2}} Y_{\nu_l}(\lambda r) Y^{lm}(\Omega) \quad (35)$$

$$\Psi_B^{lmE} = r^{-\frac{1}{2}} K_{\nu_l}(\lambda r) Y^{lm}(\Omega) \quad (36)$$

$$\lambda = \sqrt{2\mu|E|}, \quad \nu_l = \sqrt{\frac{1}{4} + j(j+1) - c},$$

where Ψ_N^{lmE} and Ψ_S^{lmE} are the solutions for $E > 0$ and Ψ_B^{lmE} is the only solution for $E < 0$. Ψ_S^{lmE} and Ψ_B^{lmE} are still singular at the origin; nevertheless, because the sphere $r < r_0$ is no longer a part of our space, the singularity of solutions at $r = 0$ is no longer important: All of the $E < 0$ solutions can be normalized, and all of the $E > 0$ solutions can be δ -function normalized. Now we wish to select those solutions that are consistent with probability conservation. Probability is conserved at the boundary $r = r_0$ if

$$\int d\Omega \left[\psi^* \frac{\partial}{\partial r} \psi - \psi \frac{\partial}{\partial r} \psi^* \right] \Big|_{r_0} = 0. \quad (37)$$

To ensure this, we impose the most general boundary condition at $r = r_0$ that is consistent with (37) by introducing a function $g_{r_0}(\Omega, \Omega')$:

$$\frac{\partial}{\partial r} \psi(r, \Omega) \Big|_{r_0} = \int d\Omega' g_{r_0}(\Omega, \Omega') \psi(r_0, \Omega') \quad (38)$$

with the requirement that $g_{r_0}(\Omega, \Omega')$ is Hermitian, i.e.,

$$g_{r_0}^*(\Omega', \Omega) = g_{r_0}(\Omega, \Omega'). \quad (39)$$

We allow the boundary condition to have a continuous dependence on r_0 through the explicit appearance of the subscript r_0 in (38) and (39). If $g_{r_0}(\Omega, \Omega')$ and $\psi(\vec{x})$ are expanded in spherical harmonics as

$$g_{r_0}(\Omega, \Omega') = Y_{lm}(\theta, \phi) g_{r_0}^{lm'l'm'} Y_{l'm'}^*(\theta', \phi') \quad (40)$$

$$\psi(\vec{x}) = \psi^{lm}(r) Y_{lm}(\theta, \phi), \quad (41)$$

then (38) and (39) take on the matrix form

$$\frac{d}{dr} \psi^{lm}(r) \Big|_{r_0} = g_{r_0}^{lm'l'm'} \psi^{l'm'}(r_0) \quad (42)$$

$$g_{r_0}^{l'm'lm*} = g_{r_0}^{lm'l'm'}. \quad (43)$$

Now, to construct the eigenfunctions of the Hamiltonian, we simply take the linear combinations of the above solutions for a given energy E which are consistent with the boundary condition. The above procedure is self-contained and distinct from the von Neumann procedure. It describes a boundary condition that restricts wavefunctions from the entire Hilbert space to a subspace on which probability is conserved at the origin. To make contact with the von Neumann procedure, we seek a relation between the boundary condition (42) and the unitary matrix that needs to be specified to apply the von Neumann theory. Instead of imposing the boundary condition (38) on all solutions to the eigenvalue equation, we can choose a particular self-adjoint extension H_U . To construct H_U , start with H_1 , the operator with the functional form of H in (33) and domain consisting of functions ψ in the Hilbert space such that $H\psi$ is in the Hilbert space. Then, create a new operator H_2 as we did in (19) and look at the solutions to the equation $H_1\phi_{\pm} = \pm i\mu\phi_{\pm}$. This time, we obtain a solution

$$\phi_{\pm}^{lm}(\vec{x}) = \phi_{\pm}^{lm}(r)Y_{lm}(\theta, \phi) \quad (\text{no sum}) \quad (44)$$

for each l, m . Since there are infinitely many l, m , n_+ and n_- are infinite, and we can create a self-adjoint operator H_U by extending the domain of H_2 to include the infinite collection of vectors $\{\phi^{lm}(\vec{x})\}$, where each vector is of the form

$$\phi^{lm}(\vec{x}) = \phi_+^{lm}(\vec{x}) + U_{l'm'}^{lm}\phi_-^{l'm'}(\vec{x}) \quad (45)$$

and where U is an infinite-dimensional unitary matrix. (Again, the ϕ^{lm} are not angular momentum components in the sense of (40) and (41).) We now seek a relationship between $U_{l'm'}^{lm}$ and $g_{r_0}^{lml'm'}$. Enforcing the hermiticity condition, $(\phi^{lm}, H_U\psi) = (H_U\phi^{lm}, \psi)$, for all ψ in the domain of H_U , we have

$$\begin{aligned} \int_{r \geq r_0} d^3\vec{x} \phi^{lm*}(\vec{x}) H_U \psi(\vec{x}) &= \int_{r \geq r_0} d^3\vec{x} (H_U \phi^{lm}(\vec{x}))^* \psi(\vec{x}) \\ \Leftrightarrow \text{Im} \int d\Omega \phi^{lm*}(\vec{x}) \left. \frac{\partial \psi(\vec{x})}{\partial r} \right|_{r_0} &= \text{Im} \int d\Omega \left. \frac{\partial \phi^{lm*}(\vec{x})}{\partial r} \right|_{r_0} \psi(\vec{x}) \end{aligned} \quad (46)$$

using the explicit functional form of the Hamiltonian, (33). Expanding ψ as in (41), we can take advantage of the orthogonality of the angular momentum harmonics to integrate them out, leaving only the radial part of the angular momentum components:

$$\begin{aligned}
& \sum_{l'm'} \left(\phi_+^{lm}(r) \delta_{l'm'}^{lm} + U_{l'm'}^{lm} \phi_-^{l'm'}(r) \right)^* \frac{d\psi^{l'm'}(r)}{dr} \Big|_{r_0} \\
&= \sum_{l'm'} \frac{d}{dr} \left(\phi_+^{lm}(r) \delta_{l'm'}^{lm} + U_{l'm'}^{lm} \phi_-^{l'm'}(r) \right)^* \psi^{l'm'}(r) \Big|_{r_0} \quad (\text{no sum on } lm). \tag{47}
\end{aligned}$$

(The “Im” of (46) has been dropped since the phase of ψ is arbitrary.) We define

$$a^{lm'l'm'}(r) = \left(\phi_+^{lm}(r) \delta_{l'm'}^{lm} + U_{l'm'}^{lm} \phi_-^{l'm'}(r) \right)^* \quad (\text{no sum}). \tag{48}$$

Note that $a^{lm'l'm'*}(r)$ is the $l'm'$ angular momentum component of $\phi^{lm}(\vec{x})$, i.e.,

$$\phi^{lm}(\vec{x}) = a^{lm'l'm'*}(r) Y_{l'm'}(\Omega). \tag{49}$$

Viewing a as a matrix in lm and $l'm'$ which depends on r , we can write (47) as

$$\frac{d}{dr} \psi^{lm}(r) \Big|_{r_0} = \left(a^{-1}(r) \frac{d}{dr} a(r) \right)^{lm'l'm'} \psi^{l'm'}(r) \Big|_{r_0}, \tag{50}$$

where the inverse and product inside the parentheses are a matrix inverse (but not a functional inverse with respect to r) and a matrix product. Since this is of the same form as (38),

$$g_{r_0}^{lm'l'm'} = \left(a^{-1}(r) \frac{d}{dr} a(r) \right)^{lm'l'm'} \Big|_{r_0}. \tag{51}$$

Furthermore, if we take $\psi = \phi^{l''m''}$ in (50) (so that $\psi^{lm}(r) = a^{l''m''lm*}(r)$), we have

$$\frac{d}{dr} a^{l''m''lm*}(r) = \left(a^{-1}(r) \frac{d}{dr} a(r) \right)^{lm'l'm'} a^{l''m''l'm'*}(r) \tag{52}$$

$$\iff \left(a^{-1}(r) \frac{d}{dr} a(r) \right)^\dagger = \left(a^{-1}(r) \frac{d}{dr} a(r) \right), \tag{53}$$

which shows that $g_{r_0}^{lm'l'm'}$ is Hermitian. Equation (51) is the desired link between the extension and the boundary condition. Now that we have found it, we ask what happens in the limiting case $r_0 = 0$. To this effect, first note that, for a fixed value of c , most of the singular Bessel function solutions cease to be normalizable in this limit. The same holds for the $\phi_\pm^{lm}(\vec{x})$: Since many of the $\phi_\pm^{lm}(\vec{x})$ are no longer normalizable, any self-adjoint extension defined in this section which adds non-normalizable $\phi_\pm^{lm}(\vec{x})$ to the domain of H_1 is no longer

valid. To determine which of the solutions $\phi_{\pm}^{lm}(\vec{x})$, $\Psi_N^{lmE}(\vec{x})$, and $\Psi_B^{lmE}(\vec{x})$ are still at least δ -function normalizable, we require, as in the previous section, that the coefficient of the $\frac{1}{r^2}$ term in the Hamiltonian be less than $\frac{3}{4}$. Then, our requirement becomes $l < l_{crit}$, where

$$l_{crit}(l_{crit} + 1) - c = \frac{3}{4}. \quad (54)$$

Those extensions that remain valid have U diagonal for $l \geq l_{crit}$, with entries such that the linear combinations of Ψ_N^{lmE} and Ψ_S^{lmE} within the domain of H_U are purely Ψ_N^{lmE} for $l \geq l_{crit}$. At this point, the reader may object that we are including an infinite number of vectors in these extensions while the von Neumann indices are now finite. This is not a problem, since the $\phi_{\pm}^{lm}(\vec{x})$ with $l \geq l_{crit}$ that we are including already exist within the domain of H_2 . Returning to equation (51), it follows that the only boundary conditions admissible in the $r_0 \rightarrow 0$ limit are those for which $g_{r_0}^{lm'l'm'}$ is diagonal, except possibly for the block with $l, l' < l_{crit}$ as $r_0 \rightarrow 0$. One should note that the relationship between g_{r_0} and U becomes singular as $r_0 \rightarrow 0$ due to the singularities of the $\phi_{\pm}^{lm}(r)$ in $a_{r_0}^{lm'l'm'}$. In general, finite entries in U lead to singular entries in $g_{r_0 \rightarrow 0}$. Thus, for $r_0 = 0$, it is more convenient to describe the domain of the Hamiltonian through U than through a boundary condition at the origin. However, if one asks for any physical description of the choice of extension, the formulation (42) is more valuable. It tells us, for instance how the radial flux leaving the boundary through the lm channel is related to the probability amplitudes at the boundary for each channel:

$$\begin{aligned} \mathcal{J}_{lm} &\equiv \psi^{lm*}(r) \frac{d}{dr} \psi^{lm}(r) \Big|_{r_0} \\ &= \sum_{l'm'} \psi^{lm*}(r_0) g^{lm'l'm'} \psi^{l'm'}(r_0) \quad (\text{no sum on } lm). \end{aligned} \quad (55)$$

In summary, we can deal with the singularity at the origin by removing a small sphere of radius r_0 from around the origin. When we do this, we must impose a boundary condition consistent with probability conservation, and we need a periodic function in two angular variables to describe this. With certain restrictions on the boundary condition when $r_0 = 0$, the angular momentum components of this function are in direct correspondence with the

elements of the unitary matrix required in the von Neumann theory. It is in this sense that the boundary condition is equivalent to a choice of self-adjoint extension, or alternatively, that the self-adjointness condition is equivalent to probability conservation at the boundary.

APPENDIX I

We start with a Hamiltonian of the form (6)

$$H = (\vec{\pi} \cdot \vec{r}) \frac{1}{2\mu r^2} (\vec{r} \cdot \vec{\pi}) + \frac{\{L^2 - e^2 g^2 - eg(\vec{\sigma} \cdot \hat{r})\}}{2\mu r^2}. \quad (56)$$

Using $-eg\hat{r} \cdot \vec{\sigma} = (\vec{L} - \vec{r} \times \vec{\pi}) \cdot \vec{\sigma}$, we can rewrite the contents of the curly braces as

$$\{\} = \vec{L}^2 + \vec{L} \cdot \vec{\sigma} - e^2 g^2 - (\vec{r} \times \vec{\pi}) \cdot \vec{\sigma} \quad (57)$$

$$= (\vec{L} + \frac{1}{2}\vec{\sigma})^2 - 1 - (\vec{r} \times \vec{\pi}) \cdot \vec{\sigma} + \frac{1}{4} - e^2 g^2. \quad (58)$$

Following the convention of [4] and [5], we define $K = -1 - (\vec{r} \times \vec{\pi}) \cdot \vec{\sigma}$. For an eigenstate of J^2 (where $\vec{J} = \vec{L} + \frac{1}{2}\vec{\sigma}$), this then becomes

$$\{\} = J^2 + K + \frac{1}{4} - e^2 g^2. \quad (59)$$

The eigenvalues of J^2 will be of the form $j(j+1)$ for $j = eg - \frac{1}{2}, eg + \frac{1}{2}, \dots$. We will show below that the eigenvalues of K are

$$\kappa = \pm \sqrt{(j + \frac{1}{2})^2 - e^2 g^2}. \quad (60)$$

Given this relation between the eigenvalues of K and J^2 , the operator represented by the terms in curly braces has eigenvalues $\kappa(\kappa+1)$, where κ is the eigenvalue of K . This demonstrates the equivalence of the terms in (6) and (7). Next, the vector potential (3) for the magnetic monopole has no radial component, so $\vec{\pi} \cdot \vec{r} = \vec{p} \cdot \vec{r}$ and $\vec{r} \cdot \vec{\pi} = \vec{r} \cdot \vec{p}$, where \vec{p} is just the mechanical momentum operator given by $-i\vec{\nabla}$. Thus, the first term of (6) is just the usual $-\frac{1}{2\mu} \frac{1}{r} \frac{\partial^2}{\partial r^2} r$ term. To prove (60), first write

$$(\vec{r} \times \vec{\pi}) \times (\vec{r} \times \vec{\pi}) = (\vec{L} + eg\vec{r}) \times (\vec{L} + eg\vec{r}) = \vec{L} \times \vec{L} + \frac{eg}{r}(\vec{L} \times \vec{r} + \vec{r} \times \vec{L}). \quad (61)$$

Now, \vec{L} satisfies $[L^i, V^j] = i\epsilon^{ijk}V^k$ for any vector operator that does not depend on spin coordinates, so the relations $\vec{L} \times \vec{L} = i\vec{L}$ and $\vec{L} \times \vec{r} + \vec{r} \times \vec{L} = 2i\vec{r}$ hold, and

$$(\vec{r} \times \vec{\pi}) \times (\vec{r} \times \vec{\pi}) = i(\vec{L} + 2eg\hat{r}). \quad (62)$$

If we now square the operator K , we see that

$$K^2 = 1 + 2\vec{\sigma} \cdot (\vec{r} \times \vec{\pi}) + (\vec{\sigma} \cdot (\vec{r} \times \vec{\pi}))^2 \quad (63)$$

$$= 1 + 2\vec{\sigma} \cdot (\vec{r} \times \vec{\pi}) + (\vec{r} \times \vec{\pi})^2 + i\vec{\sigma} \cdot [(\vec{r} \times \vec{\pi}) \times (\vec{r} \times \vec{\pi})] \quad (64)$$

using the identity $(\vec{\sigma} \cdot \vec{A})^2 = A^2 + i\vec{\sigma} \cdot (\vec{A} \times \vec{A})$. Making the substitution $\vec{r} \times \vec{\pi} = \vec{L} + eg\hat{r}$ ($(\vec{r} \times \vec{\pi})^2 = L^2 - e^2g^2$), this finally becomes

$$K^2 = 1 + \vec{\sigma} \cdot \vec{L} + L^2 - e^2g^2 = J^2 + \frac{1}{4} - e^2g^2. \quad (65)$$

Now, K commutes with J_z since it is a total angular momentum scalar. Therefore, we can find eigenfunctions $\Omega_{\kappa m}$ of K and J_z with respective eigenvalues κ and m . (Although we do not prove it here, these eigenfunctions are complete.) Then, from (65),

$$K^2\Omega_{\kappa m} = (J^2 + \frac{1}{4} - e^2g^2)\Omega_{\kappa m}, \quad (66)$$

which shows that $\Omega_{\kappa m}$ is also an eigenfunction of J^2 . Replacing J^2 in (66) with its eigenvalue $j(j+1)$, we then arrive at

$$\kappa^2 = j(j+1) + \frac{1}{4} - e^2g^2 = (j + \frac{1}{2})^2 - e^2g^2. \quad (67)$$

This proves (60), as long as we can show that κ takes on both positive and negative values.

The latter follows from the anticommutation of K with $(\vec{\sigma} \cdot \hat{r})$:

$$K(\vec{\sigma} \cdot \hat{r}) + (\vec{\sigma} \cdot \hat{r})K = 0, \quad (68)$$

as the reader may verify. Then, if $K\Omega_{\kappa m} = \kappa\Omega_{\kappa m}$,

$$K(\vec{\sigma} \cdot \hat{r})\Omega_{\kappa m} = -(\vec{\sigma} \cdot \hat{r})K\Omega_{\kappa m} = -\kappa(\vec{\sigma} \cdot \hat{r})\Omega_{\kappa m} \quad (69)$$

(the m value is unchanged through multiplication by $\vec{\sigma} \cdot \hat{r}$). Furthermore, it can be shown that

$$(\vec{\sigma} \cdot \hat{r})\Omega_{00} = \Omega_{00}. \quad (70)$$

So, from (69) and a phase convention that is consistent with (70),

$$\Omega_{-\kappa m} = (\vec{\sigma} \cdot \hat{r})\Omega_{\kappa m}. \quad (71)$$

APPENDIX II

The definitions of Hermitian and self-adjoint are [11]: An operator H is Hermitian if its domain is dense, meaning every state in the Hilbert space can be arbitrarily well-approximated by states in the domain, and if

$$(H\psi, \phi) = (\psi, H\phi), \quad (72)$$

for every ϕ and ψ in the domain of H . The adjoint of a densely defined operator H , denoted H^\dagger , is defined for any ψ such that there is an η for which

$$(\psi, H\phi) = (\eta, \phi), \quad (73)$$

for all ϕ in the domain of H . In this event $H^\dagger\psi = \eta$. H is self-adjoint if $H = H^\dagger$. A crucial part of this definition is that the domains of H and H^\dagger be equal. For a Hermitian H , the domain of H^\dagger is always at least as big as the domain of H , and $H^\dagger\phi = H\phi$ if ϕ is in the domain of H .

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